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Abstract

A dedicated AMS system for biochemical ^{14}C measurements is being built at Center for Accelerator Mass Spectrometry. The system is centered around a National Electrostatics Corporation Model 3SDH-1 1-MV Pelletron accelerator and is designed to accept two ion sources. The LLNL 64-sample Cs-sputter ion source with its zoom lens beam line is attached to one port of the electrostatic switching element. To insure efficient coupling of the source to the acceptance of the accelerator, ion-optics calculations of the low-energy injection beam line have been conducted; the results of which were used to determine the layout of the ion optical components of the beam line. Beam tests of the low-energy injection line show that beam behavior was accurately predicted by the calculations.

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Key Words: ion optics, computer modeling, accelerator mass spectrometry

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Introduction

Experiments have proven that accelerator mass spectrometry can be successfully applied to areas of biochemical interest, including studies of nutrition, toxicology, pharmacokinetics and human carcinogenesis [e.g., 1-4]. Such experiments were conducted at large multi-purpose accelerator facilities, mainly dedicated to the more the "traditional" fields of AMS research: geochemistry, geochronology, archeology and the environmental sciences. Recent work [5] demonstrates the feasibility of ^{14}C analysis with low terminal voltages, resulting in a much smaller system, with its attendant reduction in cost and increased ease of operation. At LLNL, the planned biochemical AMS application requires high throughput (>300 samples/day) with attomole sensitivity for such a system. Such sample rates are only possible with intense ion beams which suffer from significant space-charge effects [6]. This system was modeled and the results were experimentally confirmed to assure that optimal coupling between the ion source and the acceptance of the accelerator was achieved.

Figure 1 shows a schematic layout of the AMS system dedicated to biochemical ^{14}C measurements currently under construction at the Center for Accelerator Mass Spectrometry. The 45° electrostatic spherical analyzer (ESA) accommodates two different ion source lines and, as shown in Figure 1, the LLNL high-current cesium-sputter ion source [7] is attached through two einzel lens. This source produces high currents of C^- beams (200-250 _A) with a relatively large emittance (18.9 _ mm mrad rms at 40 keV). The two einzel lens act as a zoom telescope which allows for the nearly-arbitrary placement of a beam waist before the 45° ESA. After the beam is extracted at 40 keV and deflected 45°, the 90° injection magnet (ME/Z^2 = 2 amu-MeV) mass selects beams into a National Electrostatics Corporation Model 3SDH-1 1-MV Pelletron Accelerator. Between the two acceleration regions of the tandem is a 5 mm radius gas stripper canal. Although the accelerator was designed for 3 MeV C^{2+} operation, measurements of ≤1.2 MeV C^{+} are likely. After acceleration, the beam is momentum-analyzed with a double-focussing 90° analyzing magnet (ME/Z^2 = 28 amu-MeV) to measure ^{13}C levels and then energy-analyzed with a 90° electrostatic spherical analyzer (_ = 1 meter) before measuring ^{14}C levels with a solid-state particle detector or other counter.

Optics Calculations

Each particle in a beam can be represented by a point in 6-coordinate space of positions and momenta (x, y, z, p_x, p_y, p_z). Under certain conditions, simplifications may be made. Only the transverse coordinates (x, y, p_x, p_y) are of interest in matching a beam, propagated along the z-axis without time structure (i.e., DC), to ion-optical components. The absence of particle motion coupling between the xz and yz planes permits beam characterization solely in the (x, p_x) and (y, p_y) planes of phase space. Furthermore, if the particle's axial momentum is constant and large compared to its transverse momenta, then those components (p_x and p_y) can be replaced by the tangent values $x' = dx/dz$ and $y' = dy/dz$ of the divergence angles. Therefore, nonrelativistic ion-beams can be described by two independent planes in phase space: (x, x') and (y, y').

A (6x6) transfer matrix describes the focussing and transport properties of an ion optical element, but is similarly reduced to two independent (2x2) matrices. The calculation of a beam envelope at any point along a beam line involves the operation of any intervening transfer matrices upon the starting beam's phase space coordinates. Beam matching occurs when an initial ion beam is transported to a desired final focus through any limiting apertures.

POWERTRACE [8], which is a graphical user interface shell integrated to run the beam dynamics code, TRACE 3-D [9], was employed to perform the optics calculations described in this paper. TRACE 3-D uses transfer matrix formalism and includes a linear space-charge model to calculate, to first order, vertical, horizontal and longitudinal beam envelopes through an ion-transport system. Since TRACE 3-D was developed to model bunched beams, the initial longitudinal phase space parameters and beam current were adjusted to accurately represent the space charge fields of the continuous beam in this system. The wavelength of the radiofrequency of the time between beam bunches is set much longer than the pathlength of the beam to be modeled [10]. The ion current, longitudinal Twiss parameters and emittance of this extended beam bunch are then defined as prescribed in ref. [10].

Figure 2 shows the results of the optics calculations of the low-energy injection beam line of the biochemical ^{14}C AMS system. The two plots on top are phase space plots of the beam profile at both the initial and final positions. The virtual source position was defined to be midway between the sample and the cesium ionizer. A source emittance of 94.5 _ mm mrad (equivalent uniform) at 40 keV and Twiss parameters of _$_x$ = _$_y$ = 0 and _$_x$ = _$_y$ = 0.0668 mm / mrad were defined based on results of tests and modeling conducted on an identical source. To accurately reflect the space-charge forces inherent in a real beam, 100 _A of $^{14}C^-$ ions, with an extraction energy of

40 keV, was used as the test beam. It was propagated along the zoom lens ion source beamline, through the 45° spherical electrostatic analyzer and deflected with the 90° injection dipole magnet into the low energy column of the accelerator. The position of the final beam was defined to be at the midpoint of the gas stripper canal. The calculated beam envelope half-widths in both the horizontal (x) direction and the vertical (y) direction are plotted in the bottom half of Figure 2. Note that the size of the optical elements are not drawn to scale and in no instance does the beam extend beyond the acceptance of any aperture in the system. The final beam energy shown in this plot was 600 keV. Similar results were obtained when the voltage on the accelerator was increased to give a final beam energy of 1.2 MeV.

The low-energy column of the accelerator was divided into two different voltage gradients, with the first approximately 20% greater than the second. The entrance and exit apertures of the acceleration tube were set to zero to negate any POWERTRACE-calculated fringe field effects and a thin lens was inserted to handle the focussing properties of the gradient change at both the entrance to the accelerator and at the interface between the two voltage gradients. The focal lengths of the thin lens were determined by creating a grid-point mesh model of the acceleration column's structure using the ion-optics simulation code, SIMION 3D [11]. Ions were flown through the column and their paths were used to determine the appropriate focal lengths. It was found that the modeled focal lengths closely matched the formula [12]:

$$f = \frac{2V + \sqrt{4V^2 + 2.28V \cdot d \cdot \Delta E}}{E}$$

where, f is the lens focal length,

V is the total incoming ion energy,

d is the diameter of the entrance tube, and

ΔE is the change in the voltage gradient at the entrance.

While conducting the POWERTRACE calculations, the above formula was used in selecting the lens focal lengths whenever the initial ion extraction or the accelerator voltage was changed.

Beam Tests

The low-energy beam line through the 90° injection magnet has been assembled to test the ion-optics calculations. A beam diagnostics stub consisting of two beam profile monitors and a Faraday cup has been installed at the focal plane of the magnet. The spectrometer will not be fully assembled until a building addition is completed. Several beam profile monitors have been placed throughout the beam line and another Faraday cup has been inserted to measure total (unanalyzed) source output. Approximately 75% of 200 _A from a graphitized ANU sucrose sample was observed through the 90° injection magnet at m / q=12. This is a little less than the ~80% that has been observed with similar samples on the two other AMS ion sources currently in operation at CAMS. However, the acceptances of the optical elements on those systems are larger than those on the new line. The highest transmission is obtained by using the einzel lens to focus the beam to a rather broad waist before the 45° ESA and by keeping the beam wide as it enters the magnet before being focused down to a narrower waist at the magnet focal plane. Referring to the plot in Figure 2, this behavior closely matches the predictions of the ion optics calculations.

Conclusions

Ion-optics calculations have been performed on the low-energy injection beam line for a new AMS system currently under construction at CAMS. Initial tests of an ANU sucrose sample indicate that the coupling of the ion source to the low-energy injection line closely matches ion-optics calculations. The effects of the stripper gas on the beam profile will be experimentally investigated and the results will be used as input to ion-optics calculations of the high-energy analysis line. With the expected stripper efficiency and predicted beam transmission, this AMS system will be capable of measuring more than 300 biochemical samples per day with ^{14}C concentrations as low as 1 attomol ^{14}C / mg carbon (10^{-14} ^{14}C / C) at 3-5% precision.

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References

[1] S. R. Dueker, A. J. Clifford, M. W. Lame, H. J. Segall, B. A. Buchholz and J. S. Vogel, FASEB J 12 Part 1 Suppl. S (1998) A210.

[2] B. A. Buchholz, E. Fultz, K. W. Haack, J. S. Vogel, S. D. Gilman, S. J. Gee, B. D. Hammock, X. Y. Hui, R. C. Wester and H. I. Maibach, Anal. Chem. 71 (1999) 3519.

[3] K. T. Bogen, G. A. Keating, S. Meissner and J. S. Vogel, J. Expo. Anal. Env. Epid. 8 (1998) 253.

[4] M. R. Creek, C. Mani, J. S. Vogel and K. W. Turteltaub, Carcinogenesis 18, (1997) 2421.

[5] M. Suter, St. Jacob and H. A. Synal, Nucl. Instr. Meth. B 123, (1997) 148.

[6] R. Hutter, in: A. Septier (Ed.) Focusing of Charged Particles Vol. 2, Academic Press, New York and London (1967) p. 3.

[7] J. R. Southon and M. L. Roberts, this conference.

[8] AccelSoft Inc., Del Mar, CA 92014.

[9] K. R. Crandall and D. P. Rusthoi, Los Alamos National Laboratory Report LA-UR-97-886 (1997).

[10] G. H. Gillespie, Proceedings of the XIX International LINAC Conference, ANL-98/28 (1998) 150.

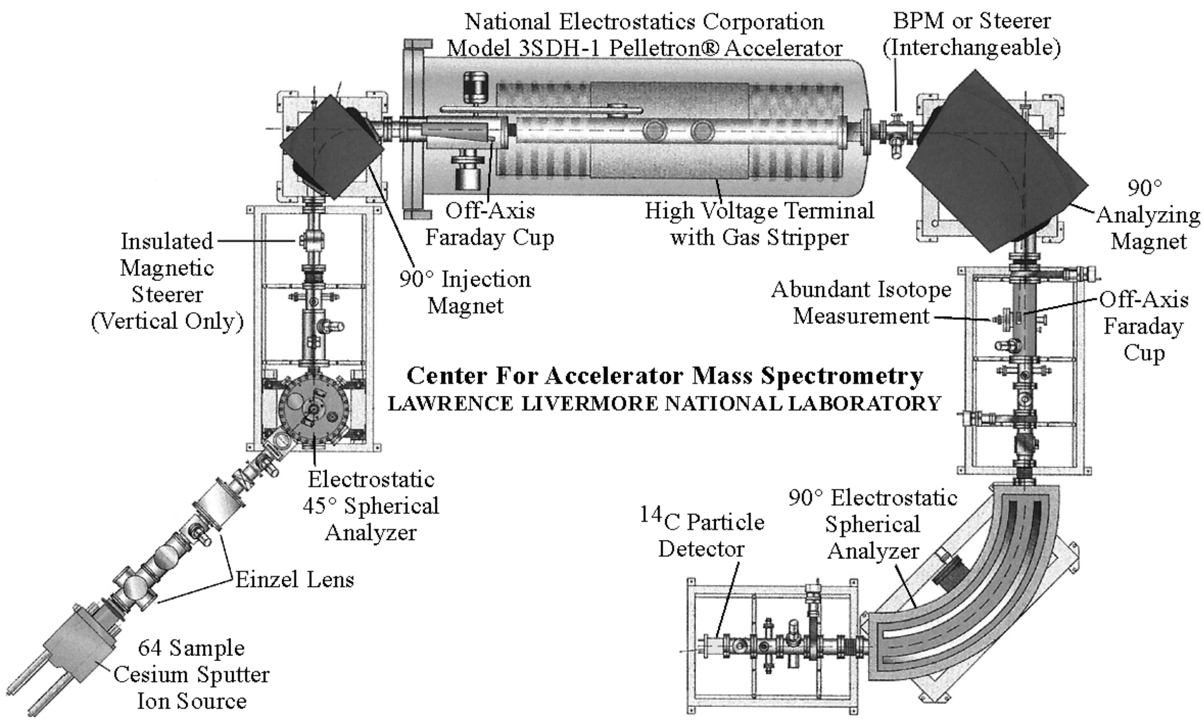
[11] D. A. Dahl, Idaho National Engineering Laboratory Report INEL-95/0403 Rev. 4 (1995).

[12] J. Ferry, National Electrostatics Corp., private communication.

Figure Captions

Figure 1. Schematic layout of the LLNL biochemical ^{14}C AMS system currently under construction at LLNL. To date, the low-energy line through the 90° injection magnet has been assembled and is undergoing beam tests.

Figure 2. Calculated phase space plots of the initial (top left) and final (top right) beam and the beam envelope half-widths plot in both the horizontal (x) and vertical (y) planes of the 40 keV $^{14}C^{-}$ test beam as it travels through the low-energy injection beam line. For this calculation, the location of the 600 keV final beam was set to the midpoint of the gas stripper canal at the center of the tandem accelerator. Note that the size of the optical elements are not drawn to scale.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Model 3SDH-1 Pelletron® Accelerator
BPM or Steerer
(Interchangeable)
90°
Analyzing
Magnet
Off-Axis
Faraday Cup
High Voltage Terminal
with Gas Stripper
Insulated
Magnetic
Steerer
(Vertical Only)
90° Injection
Magnet
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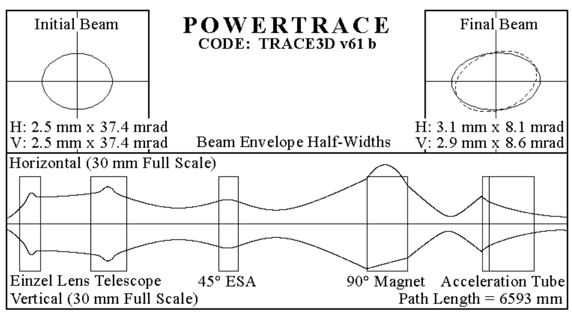
64 Sample
Cesium Sputter
Ion Source



POWERTRACE
CODE: TRACE3D v61 b
Initial Beam
H: 2.5 mm x 37.4 mrad
V: 2.5 mm x 37.4 mrad
Final Beam
H: 3.1 mm x 8.1 mrad
V: 2.9 mm x 8.6 mrad
Beam Envelope Half-Widths
Horizontal (30 mm Full Scale)
Einzel Lens Telescope
45° ESA
90° Magnet
Acceleration Tube
Vertical (30 mm Full Scale)
Path Length = 6593 mm